A study of the free energy surface of an Ising spin glass

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We study the free energy surface of a mean field model for a spin glass in a field H. We obtain field cooled and zero field cooled magnetizations that look qualitatively like experiment. The field cooled state which has the lowest free energy of any state we generated, satisfies Maxwell's relations. All states obtained by cooling have reversible properties (in the absence of relaxation effects). By contrast, any change in H below the glass transition leads to irreversibility (minima hopping), except at very large H. We have calculated hysteresis loops which compare favorably with experiment for a variety of situations and make predictions for additional hysteretic effects.

PACS numbers: 75.10.Jm, 64.60.Cn, 75.50.Kj

Spin glasses show a variety of irreversible and history dependent effects below the glass transition T_c.[1] These properties are presumably related to the existence of many metastable states. To gain an understanding of irreversibility in spin glasses, we have numerically studied the minima of the free energy surface F as a function of the average spins at each site $\{m_i\}$.

Thouless, Anderson and Palmer[2](TAP) have computed $F^{TAP}[m_i]$ for the infinite range Ising model. It appears, however, that solutions to the minimization condition $\partial F^{TAP}/\partial m_i = 0$ require using sophisticated iterative techniques[3] which involve matrix algebra. This imposes a limit on the number of particles N. Furthermore, there are unphysical minima to which the system will easily flow. Because of the difficulties associated with the TAP free energy, we considered the much simpler surface corresponding to mean field theory for Ising spins of magnitude S in a field H

$$F = 1/2 \sum_{ij} J_{ij} m_i m_j - k_B T \sum_i \ln\left[\frac{\sinh(S+1/2)\lambda_i}{\sinh \lambda_i/2}\right] \quad (1)$$

where $\lambda_i = \beta \sum_j J_{ij} m_j + \beta H$ and $-S \leq m_i \leq S$.

Here J_{ij} is the nearest neighbor exchange constant which is distributed according to

$$P(J_{ij}) = (2\pi)^{-1/2}\, \bar{J}^{-1} \exp(-J^2_{ij}/2\bar{J}^2) \quad (2)$$

We also considered the effects of adding an extra anisotropy term which enters into the Hamiltonian in the form $H^A = -\sum_i DS_i^2$ and D is the anisotropy constant. It is believed that anisotropy plays an important role in spin glasses[4,5]. We have additionally studied the case of Heisenberg spins and find that, particularly in that case, anisotropy effects must be invoked in order to obtain agreement with experimental results. In this short note we report on our findings for the case of Ising spins. Different aspects of these results have been reported elsewhere.[6]

Our system consisted of several 10x10x10 three dimensional (3d) lattices. We studied how a minimum of F evolved with H and T using an iterative approach. For each new (T,H) we started our iterations at the $\{m_i\}$ corresponding to the minimum of F evaluated at the converged values for the previous T or H. We then changed the $\{m_i\}$ using a random (updated) sequencing of the sites i until we got convergence at the n^{th} iteration defined by

$$\sum_i (m_i^n - m_i^{n-1})^2 / \sum_i (m_i^n)^2 \leq 10^{-12}.$$

For definiteness, the spin glass transition temperature T_c is defined by the lowest T at which $\sum_i m_i^2 = 0$, obtained by extrapolating to $N\to\infty$. For S=1/2, we found $T_c = 1.125\bar{J}$ and for S=5/2, $T_c = 13.0\bar{J}$. (Here $k_B \equiv 1$)

We will show here that this model, while clearly oversimplified, nevertheless, yields a number of results which are in qualitative agreement with experiment. Furthermore it makes predictions which can be checked. While fluctuation effects have not yet been included they can be superposed onto the present scheme, once the behavior of F is understood. Although our approach is numerical it is a step closer to analytical theories than Monte Carlo simulations, for it builds in the broken symmetry $m_i \neq 0$ and it allows us to check such things as the Maxwell relations (MR) which are the subject of current controversy.[7] In addition, we can readily study the degree to which two minima are correlated at any temperature and thereby deduce barrier heights.

We organize our conclusions as follows

(1) Changes in T. Any minimum which exists at temperature T_0 was found to also exist at all $T<T_0$. However, if we started with a random minimum and heated, the minimum disappeared and the system found its way to a nearby state.

(2) Changes in H. We found that changes in H were always irreversible for $H<H_R(T)$. Above H_R there is a single minimum in F. Irreversibility arises because as H is increased or decreased, minima disappear and the system finds its way to a nearby state.[6]

(3) Field Cooled (fc) state. A unique fc state is always obtained. It is insensitive to the sequencing of of $\{m_i\}$ changes, provided one starts cooling at $T>T_c$. This result was seen even in extremely weak fields. For each (H,T) this state has the lowest free energy of any state we generated. However, we did not make a systematic search. In agreement with experiment the fc magnetization is totally reversible in T.[6] Furthermore, Maxwell's relation $\partial^2 M/\partial T^2 = T^{-1}\partial C/\partial H$ (where C is the field dependent specific heat), is satisfied only in the fc case.

(4) Zero field cooled (zfc) state. The states obtained by cooling in zero field were not unique, possibly because of finite size effects. They varied depending on our choice of sequencing the changes in $\{m_i\}$. A measurement of the magnetization of a zfc state necessitates applying H below T_c and [from (2)] leads to irreversibility.

 0021-8979/82/117679-03$02.40

In Figs. 1 we plot the temperature dependence of the magnetizations M^{fc} and M^{zfc} obtained by fc (upper curves) and zfc (lower curves) processes for three different values of H. Figure 1a corresponds to spin 1/2 and 1b to spin 5/2. These spin values are defined as M_o in the figures. The curves are very similar to those

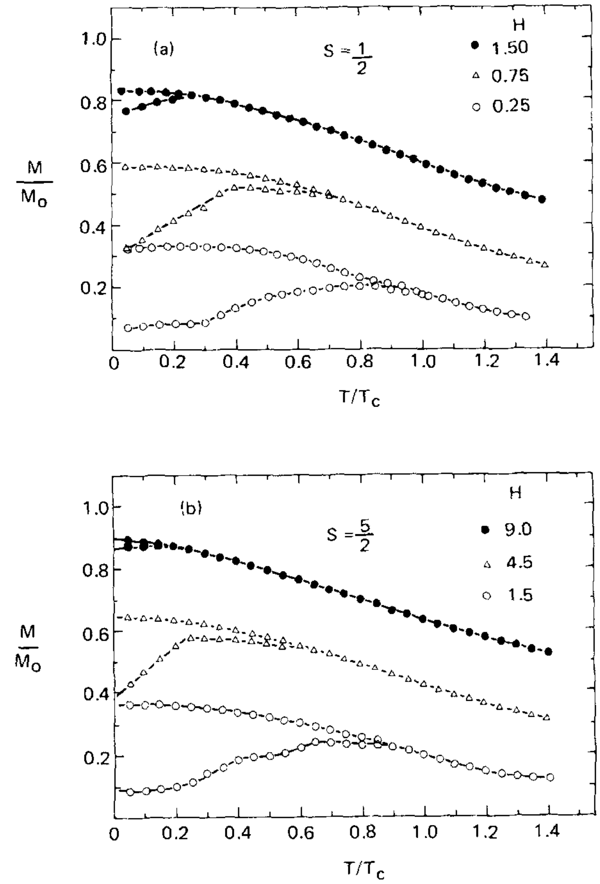

Fig. 1 Temperature dependence of the fc and zfc magnetizations for three different values of H (in units of J) for S = 1/2 (1a) and S = 5/2 (1b).

we found earlier for the 2d Ising case, except that the fc magnetization in 3d appears to be more nearly constant at low T. These results look qualitatively like those obtained experimentally: at low T, M^{fc} is nearly constant whereas M^{zfc} has a maximum at some temperature which approaches T_c as $H \to 0$. We attribute the differences between theory and experiment to finite size effects which lead to a rounding of the zfc magnetization and a smoothing out of M^{fc} as a function of temperature.

Comparing Figures 1a and 1b we see that the magnitude of the spin does not qualitatively affect the temperature dependence of the two types of magnetizations. In Fig. 2 we have plotted the fc magnetization for S=5/2 at fixed H=4J and for three values of the anisotropy constant D=0, 0.25 and 1.0 in units of T_c (evaluated at D=0). At low T/T_c, less than 0.5, we find that M^{fc} is independent of D. At higher T, the curves start to deviate; the one with the one with the largest D value corresponds to the largest magnetization.

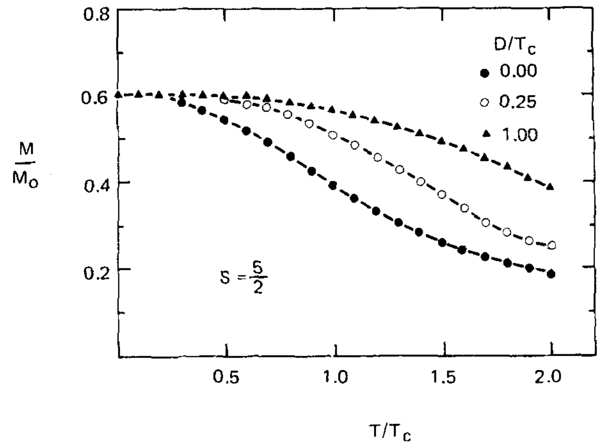

Fig. 2 Temperature dependence of the fc magnetization for three values of the anisotropy constant D, in units of T_c (evaluated at D = 0).

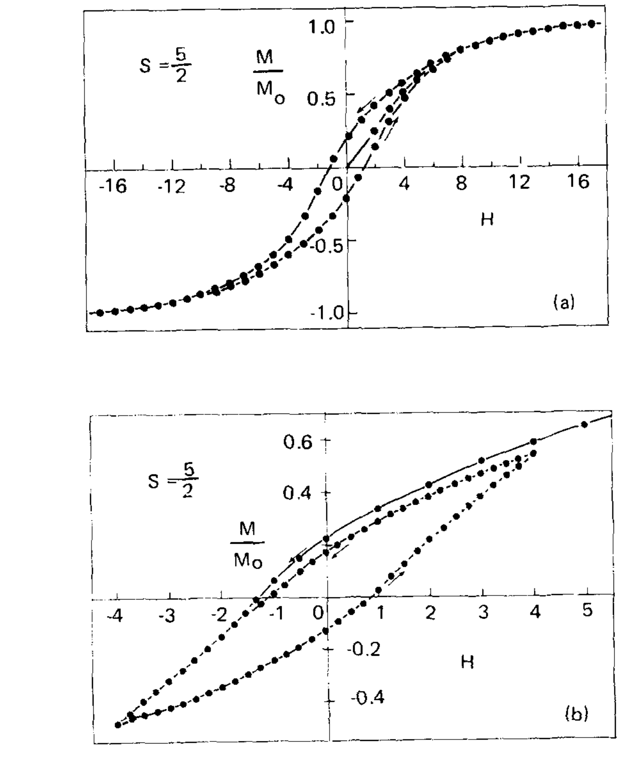

Fig. 3 Field dependence of the magnetization for a large H sweep (Fig. 3a). Fig 3b shows a displaced loop obtained after demagnetizing from large H. H is in units of J, T_c = 13.0 J and T = $0.3T_c$.

We have studied in detail the hysteresis curves for general D and S. For Ising spins they appear to be qualitatively independent of the D parameter and of the dimension of the spin glass. Figure 3a shows a hysteresis loop at $T=0.3T_c$ for $S=5/2$ for a sweep up to a large $H>H_R$. Fig. 3b shows a displaced loop obtained by first applying a large positive H, then decreasing to a small negative H and then closing the loop. Such displaced loops have been seen in field cooled AuFe spin glasses. We expect that, as in CuMn,[9] the loops obtained by initially demagnetizing from large H and by field cooling are very similar. This prediction should be checked for AuFe, whose hysteresis loop is more like that of Figs. 3 and has a rather different character than that of CuMn. We emphasize here that the hysteretic behavior we observe comes entirely from the behavior of the free energy surface. It derives from the fact that minima disappear and new ones appear as H is varied so that the systems wanders from one state to another.

ACKNOWLEDGEMENTS

We acknowledge useful conversations with M.J. Nass, D. Bowman and L.A. Turkevich and support by the NSF (DMR 81-15618) and NSF-MRL grant 79-24007.

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